



ARO Advanced Energy Conversion



Some Thoughts about the Possible Impact of Nanotechnology on Soldier Power

8 February 2001

by

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Compact Power Rationale



- Computer/radio subsystem (including GPS) requires 45.1W
- Integrated helmet and sight subsystem requires 5.6W
- Weapon subsystem (laser rangefinder, laser aiming light, thermal weapon sight, etc.) requires 6W
- Micro-climate cooling requires >100W
- Weight of non-rechargeable batteries needed for a 72-hour mission is approximately 13 lbs *without micro-climate cooling*

Source: "Energy-Efficient Technologies for the Dismounted Soldier," Committee on Electrical Power for the Dismounted Soldier, Board of Army Science and Technology, NRC Press, 1997



The 'Real-World' Customer



Photo by Sarah Underhill



The Objective Warfighter



Regardless of the uniform, the Soldier will need reliable, affordable power



SPECIFIC ENERGY (Wh/kg)

SOURCE	SPECIFIC ENERGY (Theoretical)	SPECIFIC ENERGY (Practical)
Springs (watch)	0.25	0.15
Rechargeable Batteries		35-200
Primary Li/SO ₂	1,400	175
Primary Li/SOCl ₂	1,400	300
Zinc/air		300-400
TNT	1,400	N/A
Methanol	6,200	1,500-3,100
Ammonia	8,900	1,000-4,000
Diesel (JP-8 similar)	13,200	1,320-5,000
Hydrogen	33,000	1,000-17,000
Nuclear	2,800,000	190,000

} Energy
of
Combustion

Batteries have many desirable properties (self-contained, convenient, familiar, quite safe,) and are likely to be key components of hybrid power systems



The User's Constraints

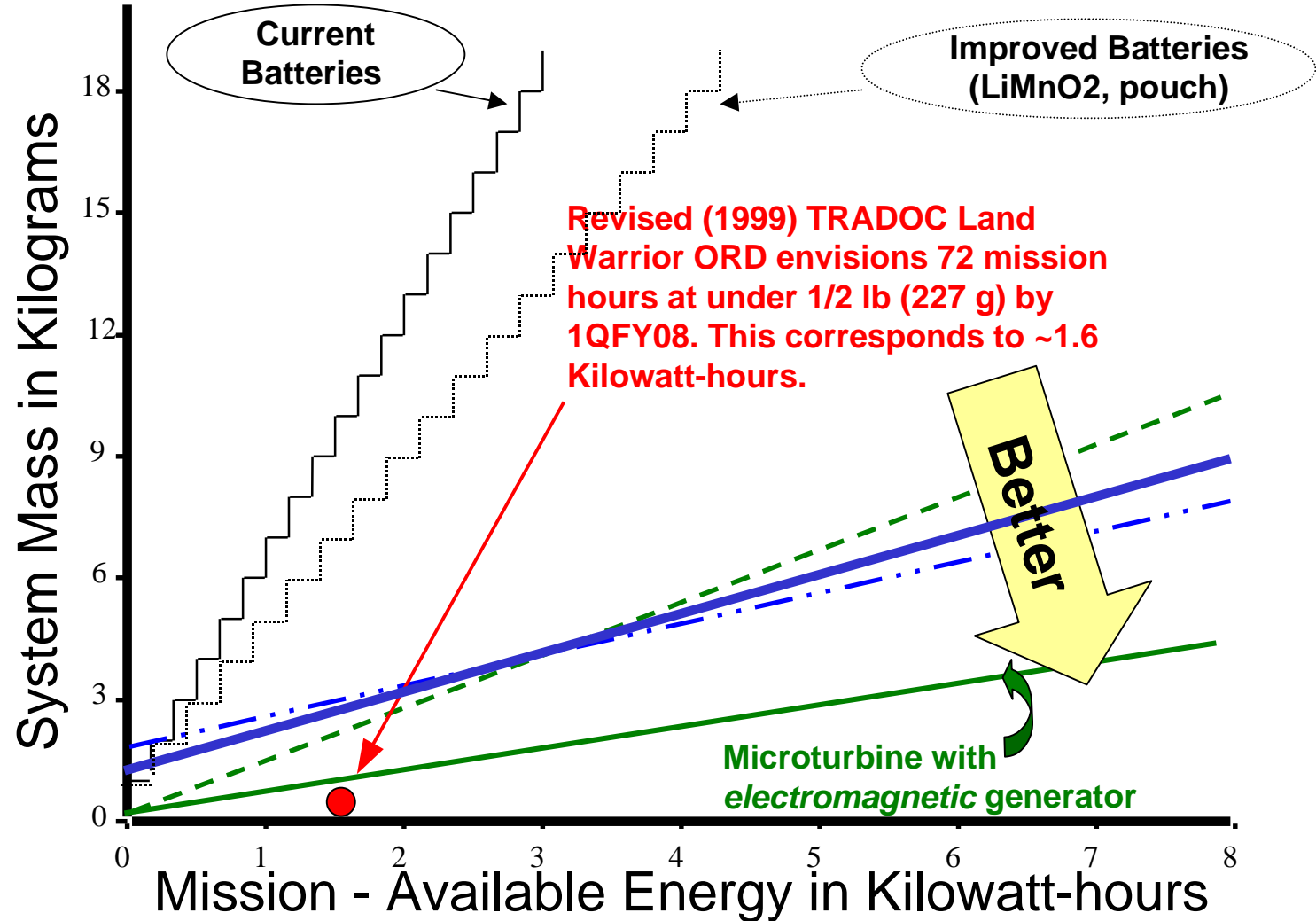
Mass-Energy Plots of Energy Conversion Systems

BA5590 Battery
1 kg device
50 W
170 Wh/kg (total)

H₂/Air Fuel Cell
0.7 kg device
15- 25 W
1 kWh/kg (fuel)

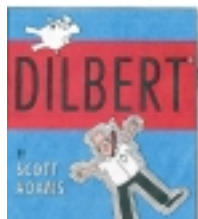
DMFC Fuel Cell
2 kg device
50-100 W
1.3 kWh/kg (fuel)

Micro gas turbine
<100 g device
50-100 W
.78 kWh/kg (fuel)





Everybody knows about batteries



From News & Observer, 8 Jan 2001



Advanced Energy Conversion Focus Areas



Electrocatalysts

Proton Conducting Membranes

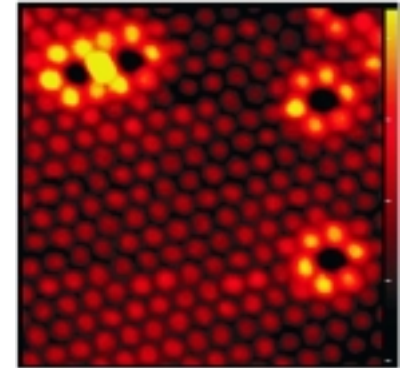
Microchemical Systems

Micro Turbine Power Systems

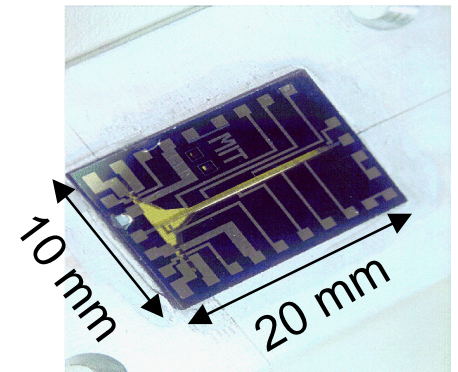
Hydrogen Sources/Storage

Hybrid Power Systems

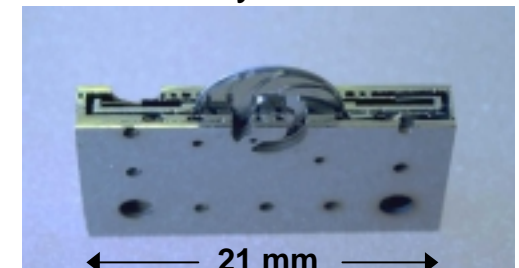
Thermophotovoltaics



Designed Catalyst - Norskov



Microchemical system - Jensen



Microturbine - Epstein



Examples in H₂/Air fuel cell evolution



- 1992 - Analytic Power - SBIR:
- 15 W (on a good day)
- No fuel included
- 5 pounds
- Short life
- Analytic Power now produces much better stacks



- 1996 - H-Power -DARPA/ARO:
- 40 W sustained
- 90 Wh of stored hydrogen
- 3.5 pounds
- Starts/runs reliably after 3+ years
- Stack is used in commercial products



- 2000?- Ball Aerospace -CECOM??:
- Concept based on available technology
- 15 W sustained, 25 W peak
- 400 Wh of generated hydrogen
- 2.2 pounds

Relative Energy Density

The big challenge is the fuel supply



Fuel cells in field exercise, Oct 1999



Ball Aerospace PPS units supporting radio retrans link at Marines CAX 1/2-99 at the 29 Palms Marine Base on 19 Oct 1999 - support for development of these fuel cells came from DARPA, ARL-ARO/SEDD, SOCOM, CECOM, and the intelligence community.

Cost of operation - \$26.18/day for fuel cells vs \$900/day for BA5590 batteries



FIGURE 1: CATALYST DESIGN FROM FIRST PRINCIPLES

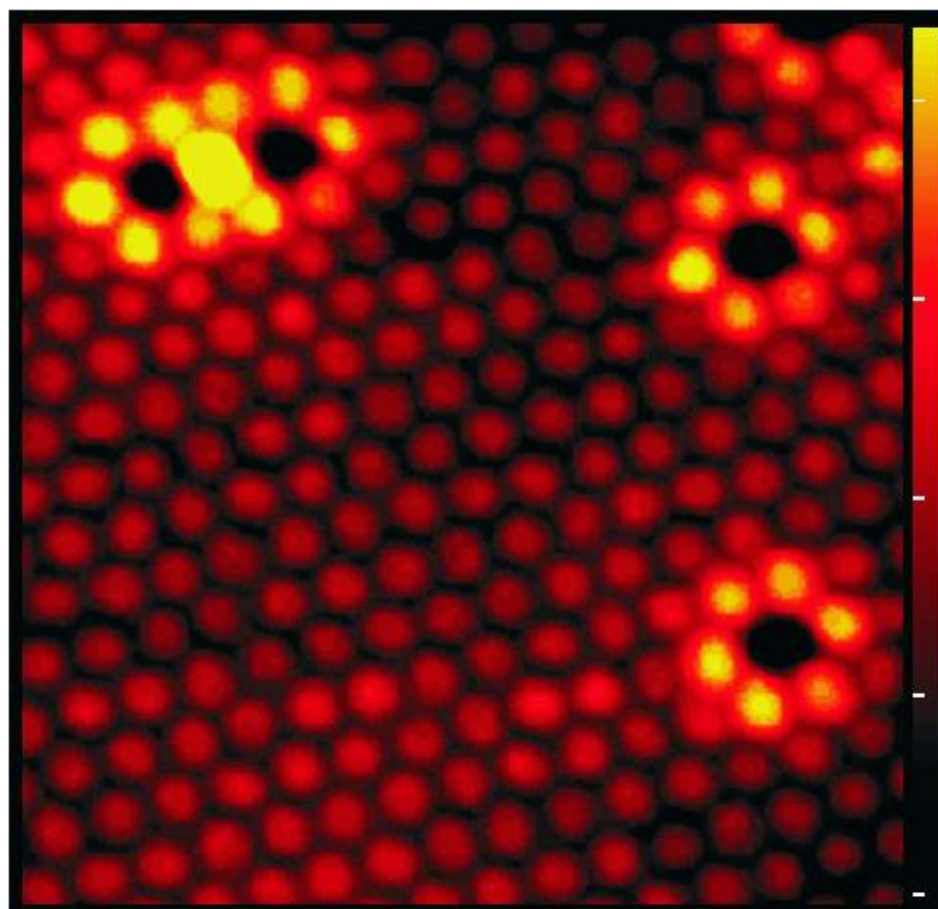


Figure 1: STM image of a Ni(111) surface with 2% of a monolayer of Au. The Au atoms appear black in the images. The Ni atoms next to the Au atoms appear brighter due to a change in geometry and electronic structure, indicating that the chemical activity of the Ni atoms may be modified by nearest neighbor Au atoms.

FIGURE 3: CATALYST DESIGN FROM FIRST PRINCIPLES

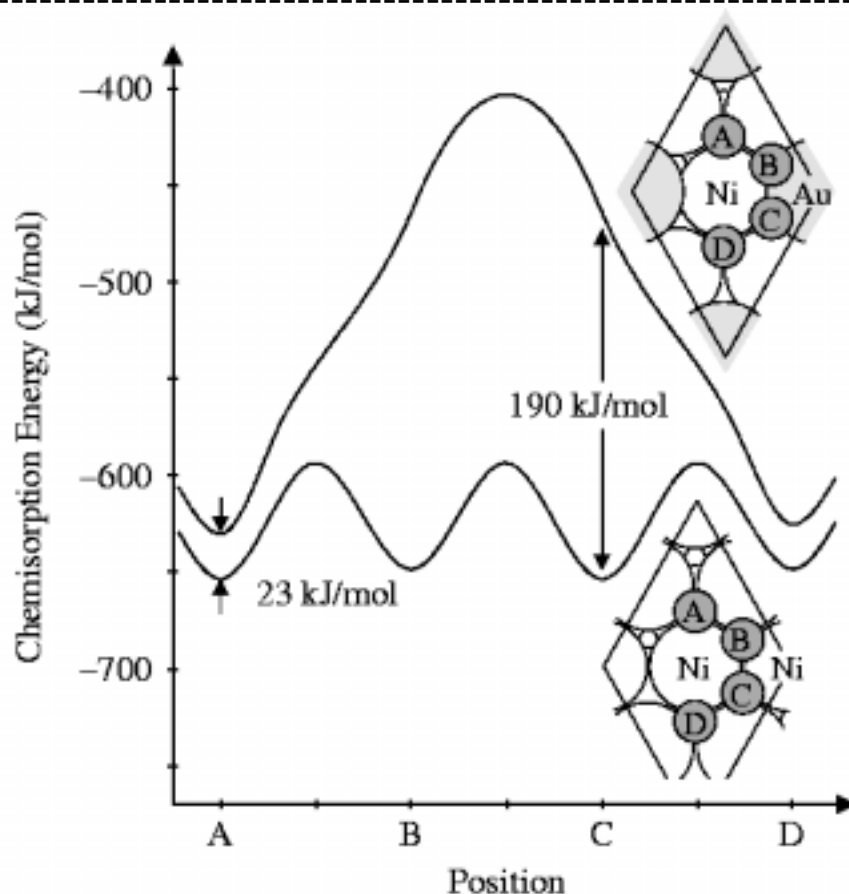


Figure 3: The calculated adsorption energy of a C atom on a Ni(111) surface as a function of position along the surface. The same energy function is shown above when one of the surface Ni atoms has been exchanged for a Au atom. The inserts show the geometry in the two cases



FIGURE 4: CATALYST DESIGN FROM FIRST PRINCIPLES

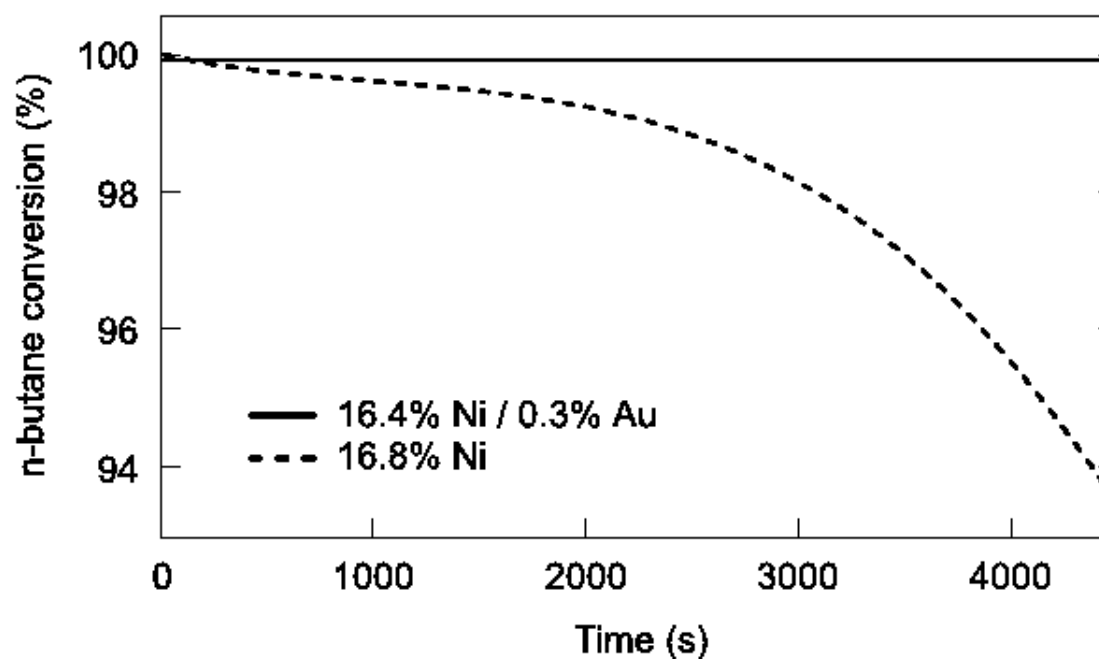
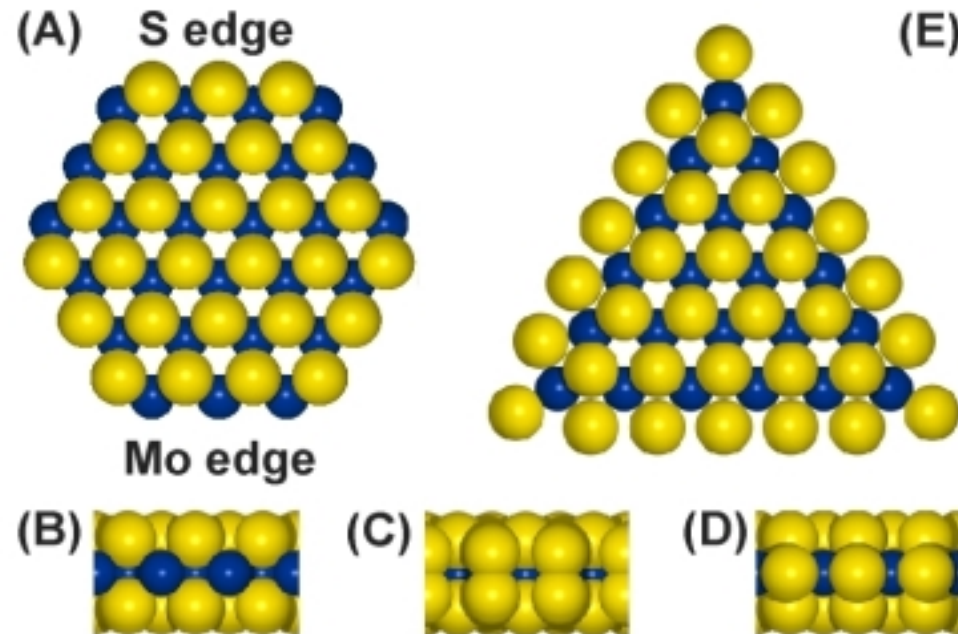


Figure 4: Conversion of n-butane as a function of time during steam reforming in a 3% n-butane-7% hydrogen-3% water in helium mixture at a space velocity of 1.2h^{-1} . The dashed curve shows the n-butane conversion for the Ni and the solid curve is for the Au/Ni supported catalyst.

ATOMIC-SCALE STRUCTURE OF SINGLE-LAYER MoS_2 NANOCUSTERS



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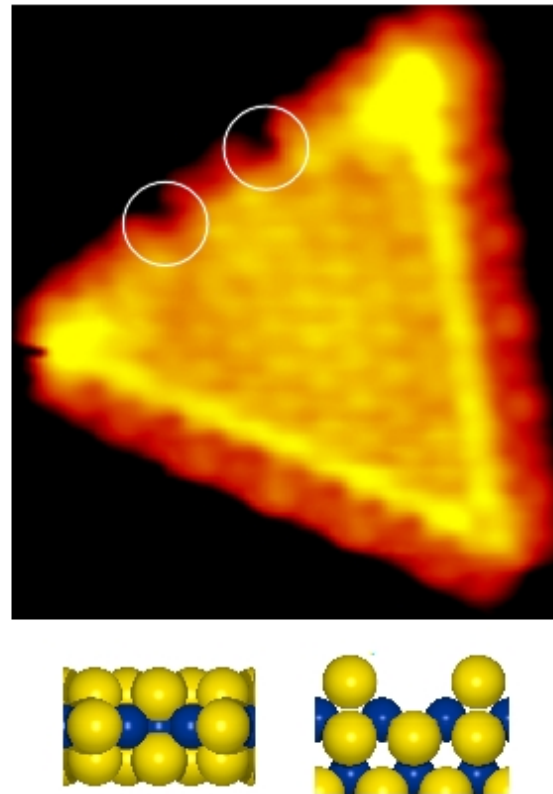
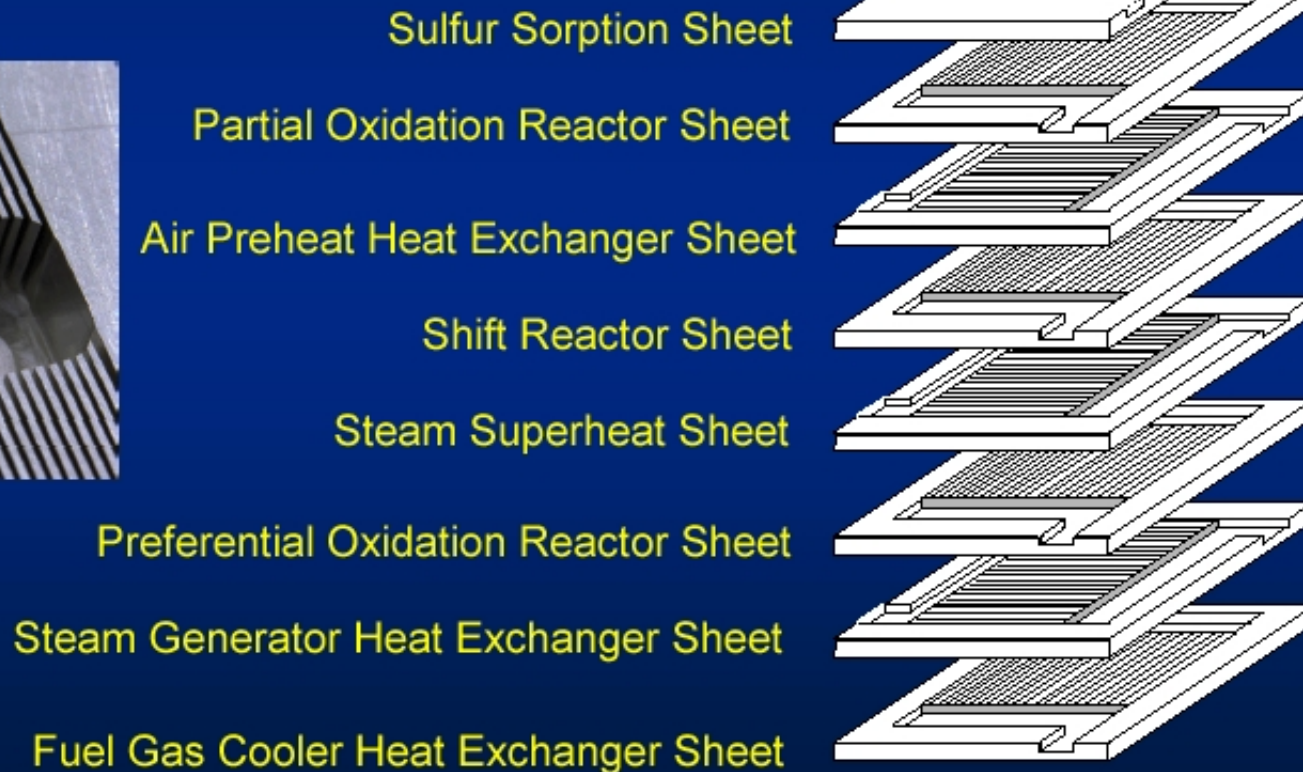
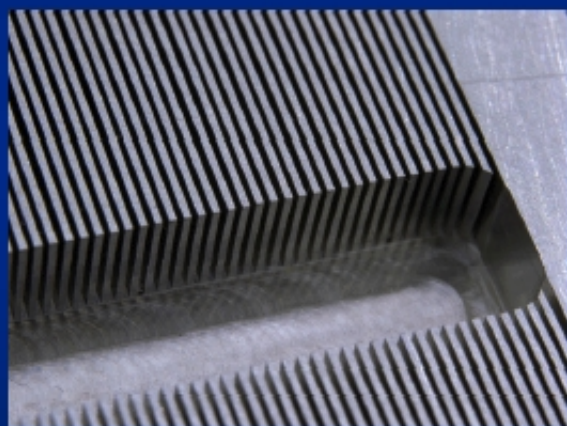


Figure 3: An atom-resolved image of a MoS_2 nanocluster exposed to atomic hydrogen which resulted in the formation of two S vacancies at the edges indicated by the white circles.

Energy Related Microreactor Efforts

- **Pacific Northwest National Laboratory (PNNL)**
 - Proposed integrated fuel processing unit for hydrogen production from liquid fuel
 - Microchannel layered device



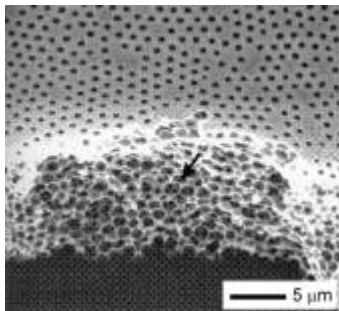


Pre-reformer

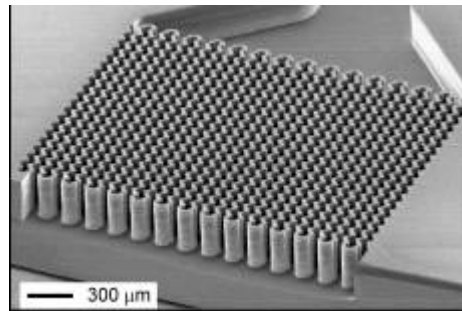


Need to get enough surface area/mass transfer to get enough reaction

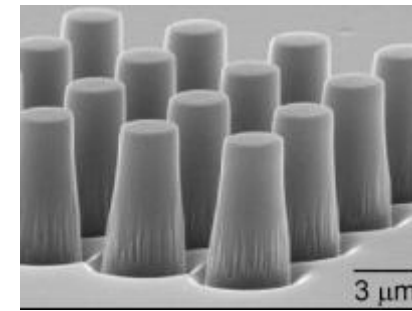
- Need to Build Appropriate Structures



Zia, et al



IMM



Adesida, UIUC

- Coat With Porous Structures to Hold Catalysts

Courtesy Prof Rich Masel, UIUC



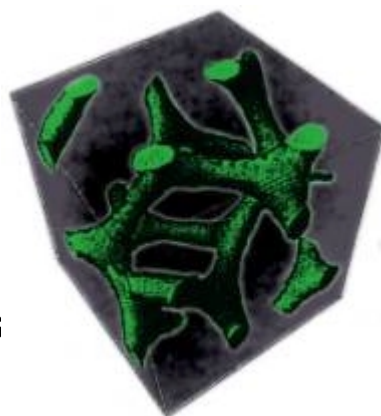
Nanotechnology useful for porous coatings



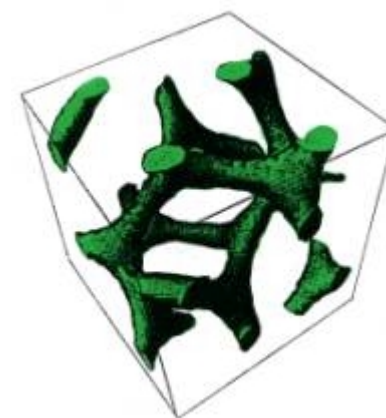
ACF



Inorganic
Precursors
Or
Nanoparticles



Calcine
And
Sinter



Porous Catalyst
Structure

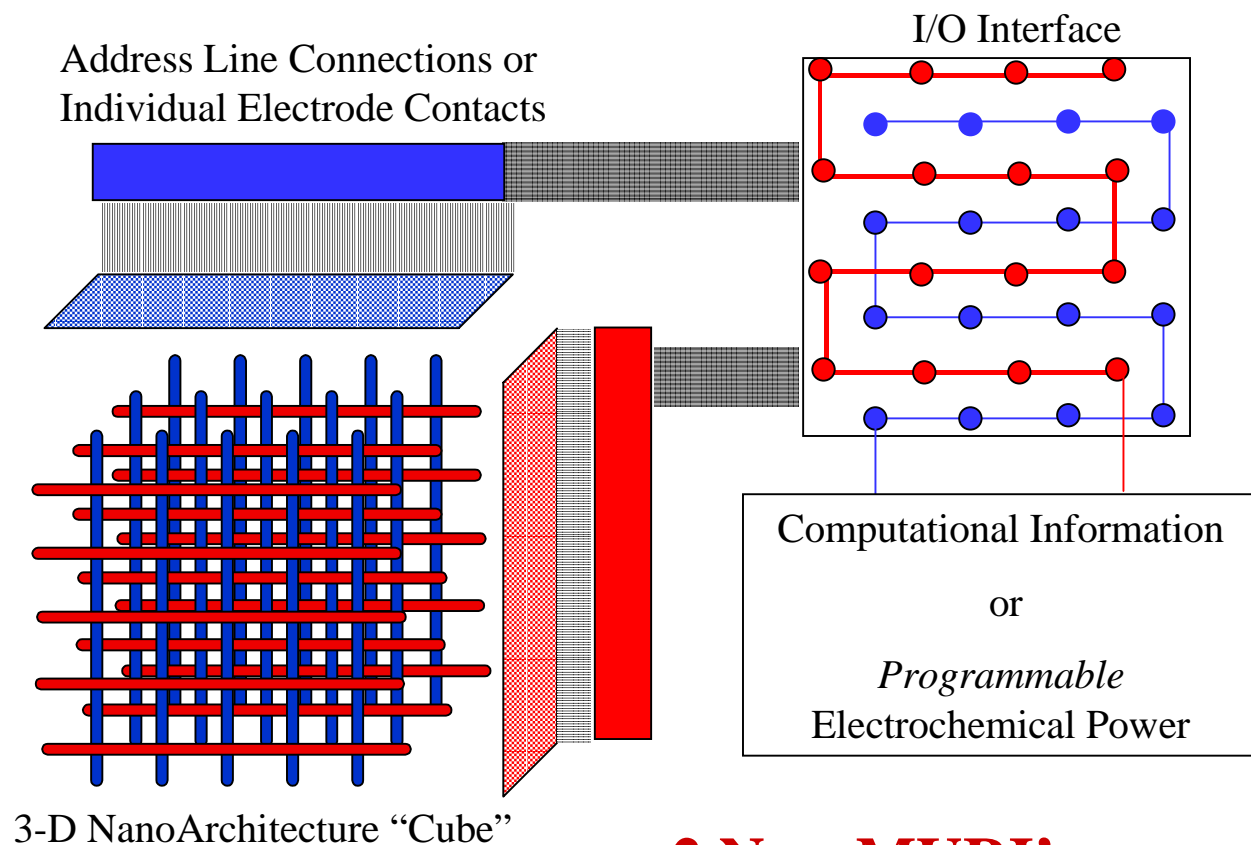
Surface=2000 m²/gm

Courtesy Jim Economy, UIUC

FY01 Multidisciplinary University Research Initiative (MURI)

3-D NanoArchitectures (D³NA) for Future Electrochemical Power Sources

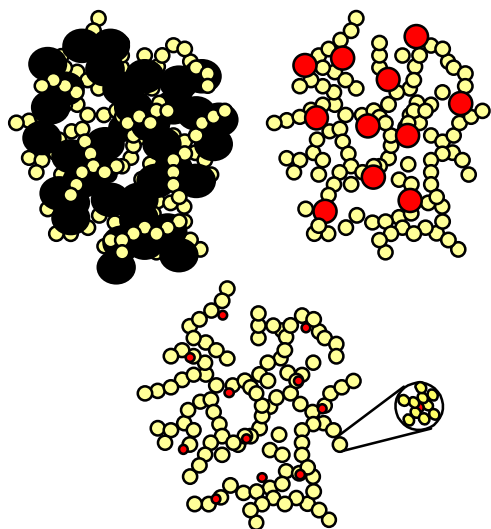
The 3-D Nanoarchitecture (D³NA) program will develop the scientific underpinnings and the basic nanostructure building blocks for revolutionary approaches to electrochemical power sources. The umbrella concept relies upon the intelligent assembly of electroactive nanometer-scale structures to construct power modules of controllable size (submicron to multi-centimeter) in a manner compatible with microelectronics and microelectromechanical systems.



2 New MURI's announced 5 Feb

Electrochemistry \Leftrightarrow Nanoscience

Exploit nanoarchitected electroactive structures & composites to enhance electrochemical performance of macro & microscale power sources while developing a comprehensive understanding of electron and ion transport at nanoscale dimensions.



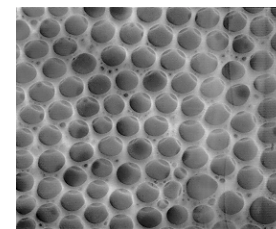
																1 H 1.00794 ± 0.00005	2 He 4.0026 ± 0.0005														
3 Li 6.941 ± 0.005	4 Be 9.0122 ± 0.0005															5 B 10.811 ± 0.003	6 C 12.0108 ± 0.0003	7 N 14.0067 ± 0.0003	8 O 15.9994 ± 0.0001	9 F 18.9984 ± 0.0005	10 Ne 20.1798 ± 0.0005										
11 Na 22.98976928 ± 0.00005	12 Mg 24.304 ± 0.0005															13 Al 26.9815385 ± 0.00005	14 Si 28.0858 ± 0.0003	15 P 30.973762 ± 0.0003	16 S 32.06 ± 0.003	17 Cl 35.453 ± 0.003	18 Ar 39.948 ± 0.0005										
19 K 39.0983 ± 0.0005	20 Ca 40.078 ± 0.003	21 Sc 44.955912 ± 0.0003	22 Ti 47.88 ± 0.003	23 V 50.9415 ± 0.0003	24 Cr 51.9961 ± 0.0003	25 Mn 54.938045 ± 0.0003	26 Fe 55.845 ± 0.003	27 Co 58.933195 ± 0.0003	28 Ni 58.6934 ± 0.0003	29 Cu 63.546 ± 0.003	30 Zn 65.38 ± 0.003	31 Ga 69.723 ± 0.003	32 Ge 72.63 ± 0.003	33 As 74.9216 ± 0.0003	34 Se 78.96 ± 0.003	35 Br 79.904 ± 0.003	36 Kr 83.80 ± 0.003														
37 Rb 85.47 ± 0.003	38 Sr 87.62 ± 0.003	39 Y 88.90584 ± 0.0003	40 Zr 91.224 ± 0.003	41 Nb 92.90638 ± 0.0003	42 Mo 95.94 ± 0.003	43 Tc 98 ± 0.003	44 Ru 101.07 ± 0.003	45 Rh 102.9055 ± 0.0003	46 Pd 106.3276 ± 0.0003	47 Ag 107.8682 ± 0.0003	48 Cd 112.411 ± 0.0003	49 In 114.818 ± 0.0003	50 Sn 118.710 ± 0.0003	51 Sb 121.757 ± 0.0003	52 Te 127.603 ± 0.0003	53 I 126.90549 ± 0.0003	54 Xe 131.29 ± 0.003														
55 Cs 132.90545196 ± 0.00005	56 Ba 137.327 ± 0.003	57 La 138.90471 ± 0.0003	58 Ce 140.12 ± 0.003	59 Pr 140.90765 ± 0.0003	60 Nd 144.242 ± 0.0003	61 Pm 144.91274 ± 0.0003	62 Sm 150.36 ± 0.003	63 Eu 151.964 ± 0.0003	64 Gd 157.25 ± 0.003	65 Tb 158.92535 ± 0.0003	66 Dy 162.5001 ± 0.0003	67 Ho 164.93032 ± 0.0003	68 Er 167.259 ± 0.003	69 Tm 168.93274 ± 0.0003	70 Yb 173.05468 ± 0.0003	71 Lu 174.967 ± 0.003	72 Hf 178.49 ± 0.003	73 Ta 180.94788 ± 0.0003	74 W 183.84 ± 0.003	75 Re 186.207 ± 0.003	76 Os 190.23 ± 0.003	77 Ir 192.222 ± 0.003	78 Pt 195.083 ± 0.003	79 Au 196.966569 ± 0.0003	80 Hg 200.59 ± 0.003	81 Tl 204.3833 ± 0.0003	82 Pb 207.2 ± 0.003	83 Bi 208.9804 ± 0.0003	84 Po 209 ± 0.003	85 At 210 ± 0.003	86 Rn 222 ± 0.003
87 Fr [223]	88 Ra [226]	89 Ac [227]	90-104															105-118													

Anderson, Stroud, Morris, Merzbacher, Rolison, *Adv. Engineer. Mater.*

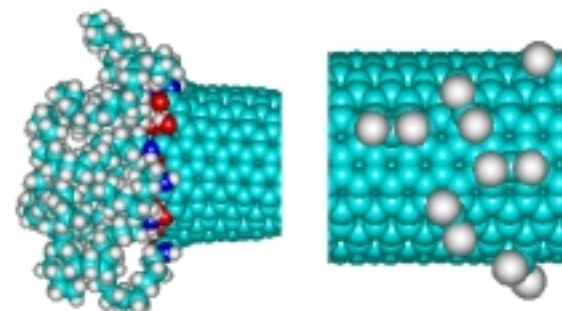


Nanoscience for the Marine 2010

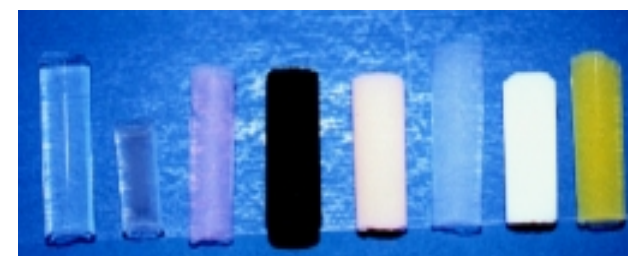
- NanoArchitected Power Sources for Electronics & Pulsed Weapons
- Aerogel Nanocomposites for CBW Sensors & Filters
- Photonic Bandgap Face Shield Coatings for Laser Protection
- Carbon Nanotube for Lightweight Armor & Nanoelectronics
- Nanoporous Polymers for CBW & Environmental Protective Clothing



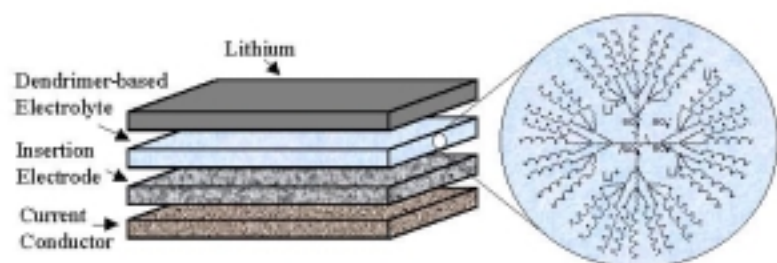
Photonic Bandgap Polymer



Derivatized Carbon Nanotubes



Silica Aerogel Nanocomposites

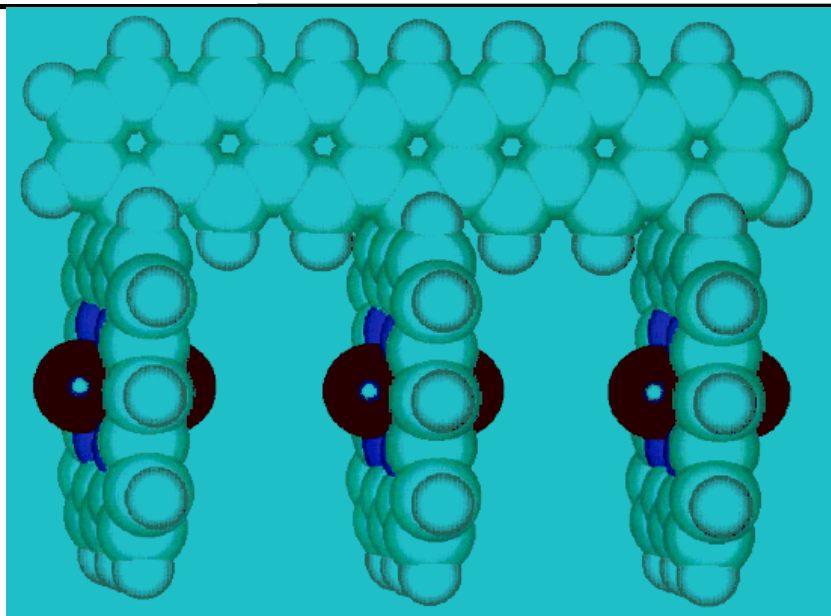


*NanoArchitected
Lithium Battery*



Low Dimensional Fast Ion Conductor

Larry Scanlon, AFRL/PO



PURPOSE

- Design and build a single lithium ion conducting polymer electrolyte with a high conductivity (~ 1 mS/cm) over a broad temperature range (+70 to -30°C) that is to be used in the construction of a rechargeable lithium polymer battery
- High electrode electrochemical stability especially at the lithium anode

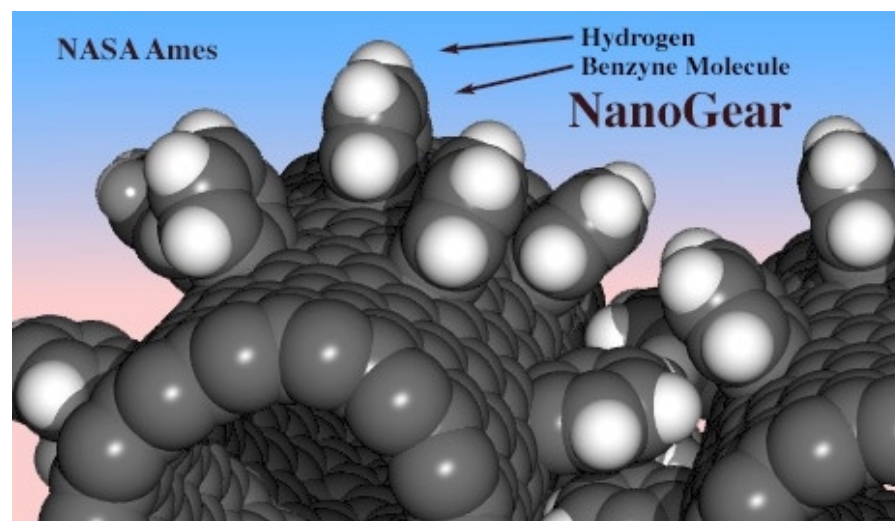
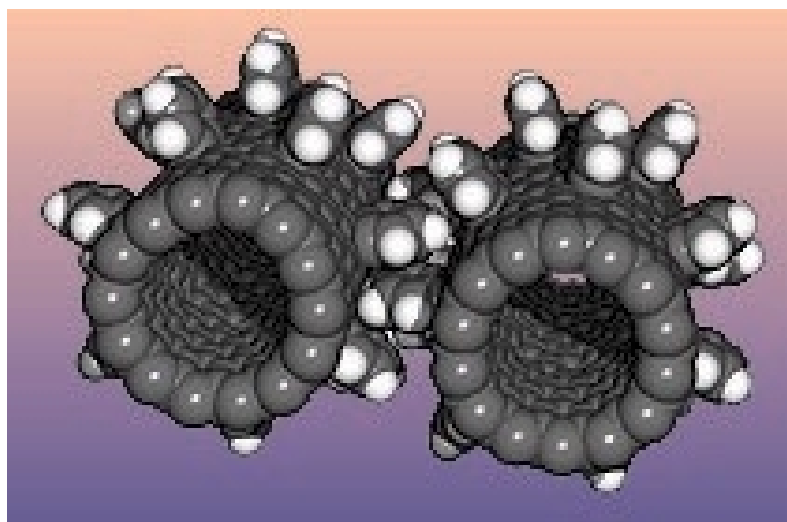
APPROACH

- Molecular orbital calculations were used to design a single Li-ion conducting channel with a constant solvent coordination sphere for lithium ions
- Unsaturated macrocyclic ring is important for achieving high lithium electrode/electrolyte interfacial stability

DOD TECH PAYOFF

- Dramatic reduction in percentage of battery weight on satellites and UAV
- Hybrid energy store for burst power applications

Molecular Dynamics Simulations of Carbon Nanotube Based Gears
Jie Han and Al Globus, MRJ, Inc., Richard Jaffe, NASA, and Glenn Deardorff, Sterling Software
NASA Ames Research Center, Moffett Field, CA 94035



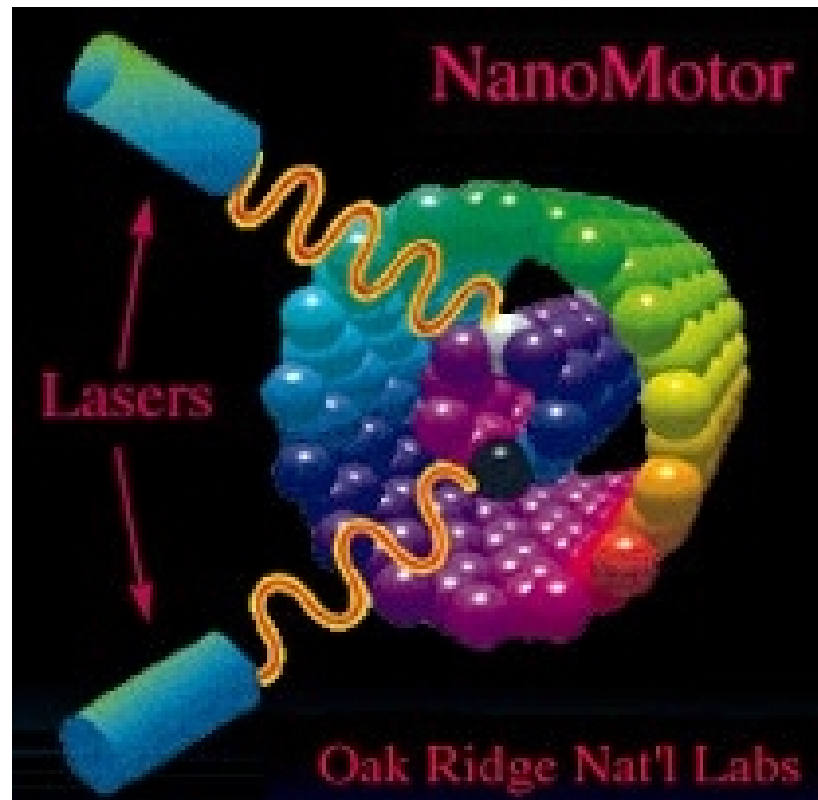
"Results suggest these gears can operate at up to 50-100 gigahertz in a vacuum or inert atmosphere at room temperature. The failure mode involves tooth slip, not bond breaking, so failed gears can be returned to operation by lowering temperature and/or rotation rate."

Abstract

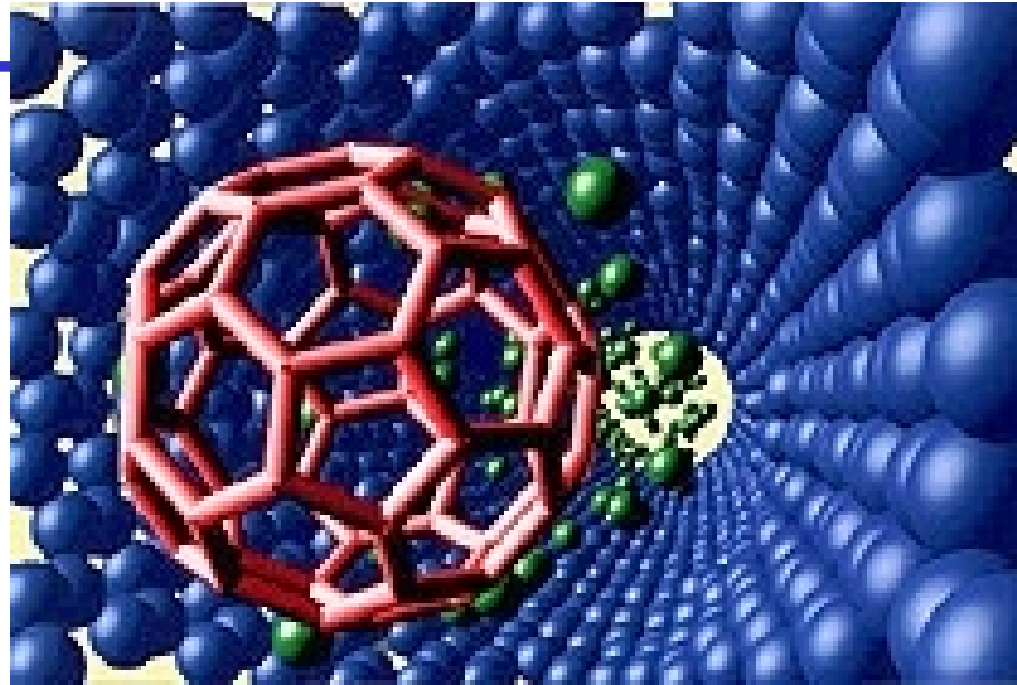
We used molecular dynamics to investigate the properties and design space of molecular gears fashioned from carbon nanotubes with teeth added via a benzyne reaction known to occur with C60 [Hoke 92]. A modified, parallelized version of Brenner's potential [Brenner 90] was used to model interatomic forces within each molecule. A Leonard-Jones 6-12 potential [Allen 87] was used for forces between molecules. One gear was powered by forcing the atoms near the end of the buckytube to rotate, and a second gear was allowed to rotate by keeping the atoms near the end of its buckytube on a cylinder. The meshing aromatic gear teeth transfer angular momentum from the powered gear to the driven gear. A number of gear and gear/shaft configurations were simulated. Cases in vacuum and with an inert atmosphere were examined. In an extension to molecular dynamics technology, some simulations used a thermostat on the atmosphere while the hydrocarbon gear's temperature was allowed to fluctuate. This models cooling the gears with an atmosphere. Results suggest that these gears can operate at up to 50-100 gigahertz in a vacuum or inert atmosphere at room temperature. The failure mode involves tooth slip, not bond breaking, so failed gears can be returned to operation by lowering temperature and/or rotation rate.

See Full paper at.....

http://www.nas.nasa.gov/Groups/Nanotechnology/publications/MGMS_EC1/simulation/paper.html



"The motors consisted of two concentric graphite cylinders (shaft and sleeve) with one positive and one negative electric charge attached to the shaft. Rotational motion of the shaft was induced by applying one or sometimes two oscillating laser fields. The shaft cycled between periods of rotational pendulum-like behavior and unidirectional rotation (motor-like behavior). The motor on and off times strongly depended on the motor size, field strength and frequency, and relative location of the attached positive and negative charges."



NanoPipes... Buckytubes, the multi-use nano component grow to different diameters and conduct electricity like copper, even better when stuffed with metal atoms. Larger tubes are big enough to pipe full sized C60 Buckyball molecules as in the illustration of the soccer ball shape (red) followed by Helium atoms (green), used as a transport "fluid". In addition to piping atoms and molecules, for perhaps a nanomachine construction sites, these tubes could be used as ultra small chemical reaction vessels.



Odds and Ends



- Fuel Cell interfaces
 - Fuel transport to catalyst
 - Ion mobility away from catalyst to electrolyte
 - Electron mobility away from catalyst to current collector
 - ‘Exhaust’ product transport away from catalyst (CO in DMFCs)
- Nanofluidics
 - Ion channels, biomimetics